



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZT6  
Title : GLGE ISOFORM 1 FROM STREPTOMYCES COELICOLOR WITH  
ALPHA-CYCLODEXTRIN AND MALTOSE BOUND  
Authors : Syson, K.; Stevenson, C.E.M.; Rejzek, M.; Fairhurst, S.A.; Nair, A.; Bruton,  
C.J.; Field, R.A.; Chater, K.F.; Lawson, D.M.; Bornemann, S.  
Deposited on : 2011-07-01  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

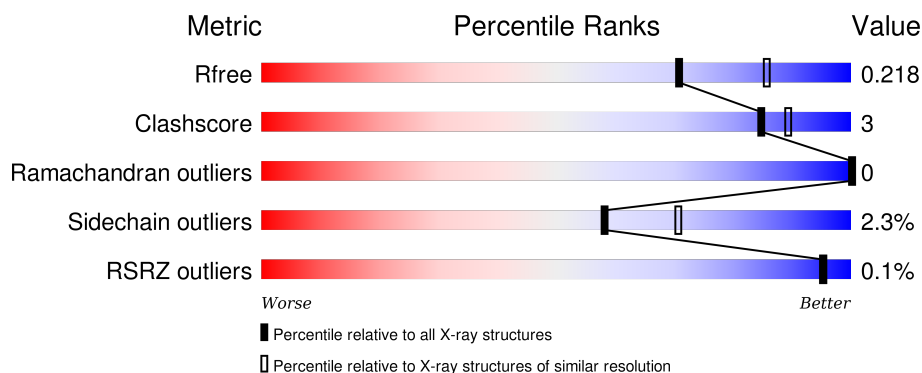
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	695	 86% 7% 7%
1	B	695	 87% 6% 7%
1	C	695	 85% 8% 7%
1	D	695	 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACX	A	701	-	-	-	X
2	ACX	B	701	-	-	-	X
2	ACX	C	701	-	-	-	X
2	ACX	D	701	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21210 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PUTATIVE GLUCANOHYDROLASE PEP1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5105	3228	922	945	10			
1	B	649	Total	C	N	O	S	0	0	0
			5093	3222	915	946	10			
1	C	649	Total	C	N	O	S	0	0	0
			5102	3228	921	943	10			
1	D	649	Total	C	N	O	S	0	0	0
			5095	3222	918	945	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
A	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
A	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
A	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
A	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
A	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2

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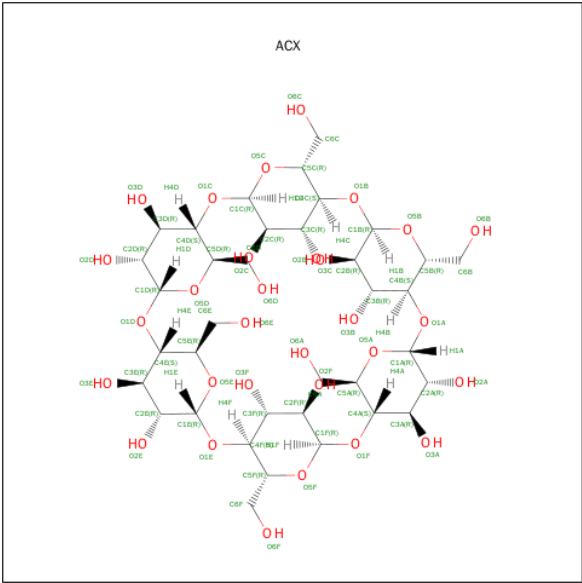
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
B	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
B	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
B	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
C	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
C	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
C	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
C	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
D	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
D	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
D	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
D	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2

- Molecule 2 is SUGAR (ALPHA-CYCLODEXTRIN (CYCLOHEXA-AMYLOSE)) (three-letter code: ACX) (formula: C<sub>36</sub>H<sub>60</sub>O<sub>30</sub>).



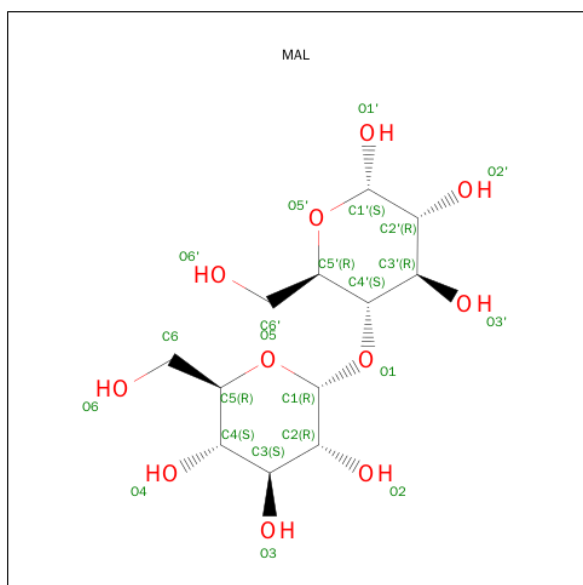
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			66	36	30		
2	B	1	Total	C	O	0	0
			66	36	30		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			66	36	30		
2	D	1	Total	C	O	0	0
			66	36	30		

- Molecule 3 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	111	Total	O	0	0
			111	111		
4	C	120	Total	O	0	0
			120	120		

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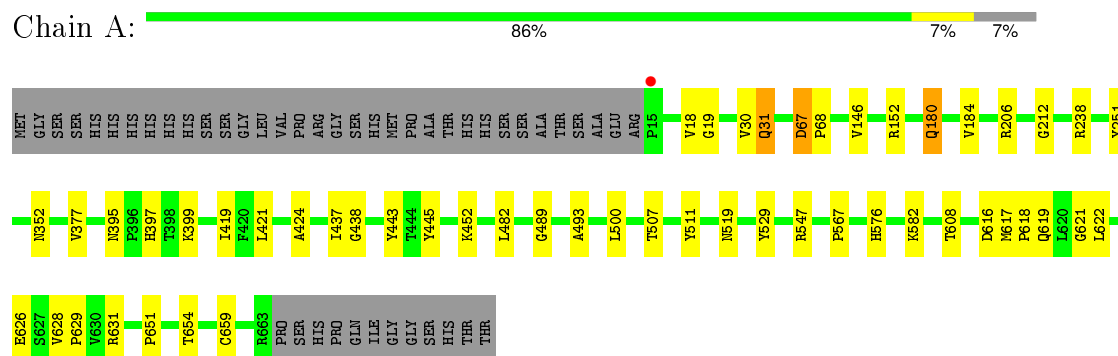
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	101	Total	O	0	0
			101	101		



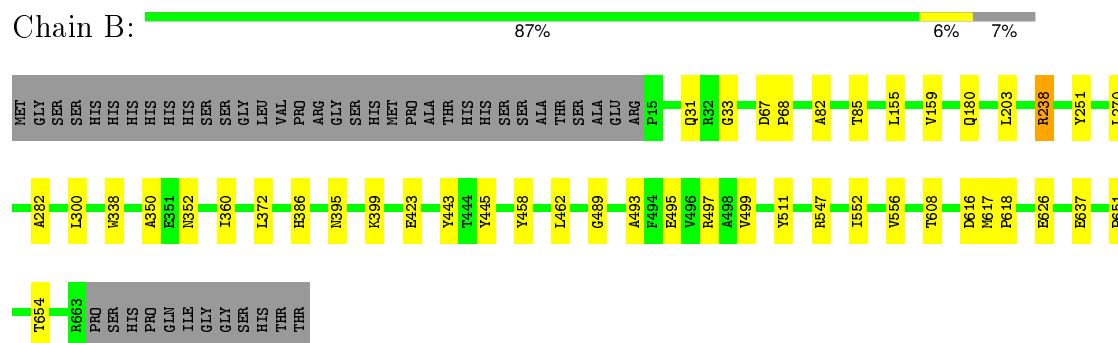
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

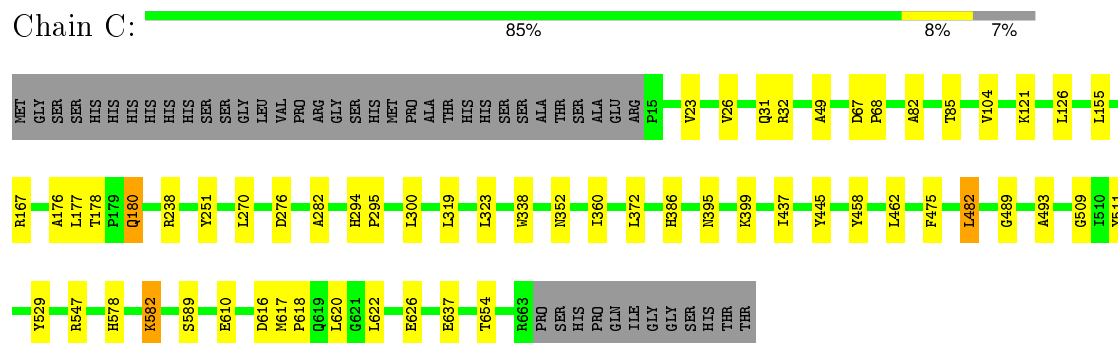
- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A



- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A



- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A



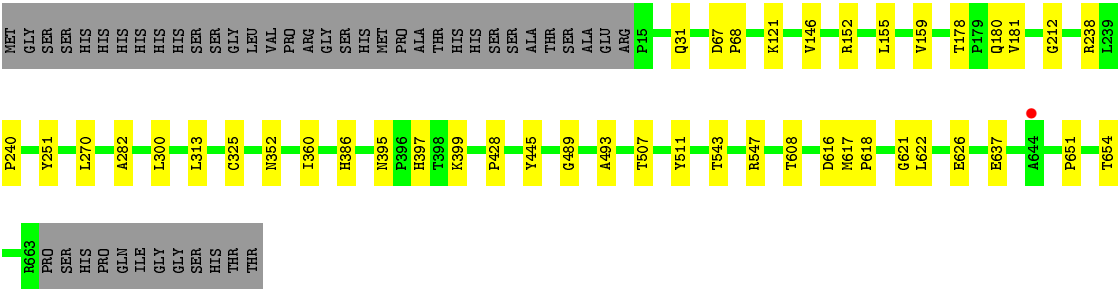
- Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A

Chain D: 

87%

6%

7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.85Å 114.16Å 315.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.39 – 2.19 56.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (56.39-2.19) 97.9 (56.39-2.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.208 , 0.236 0.199 , 0.218	Depositor DCC
$R_{free}$ test set	10297 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 0.5	EDS
Estimated twinning fraction	0.514 for H,K,L 0.486 for K,H,-L 0.457 for k,h,-l	Xtriage
Reported twinning fraction	0.514 for H,K,L 0.486 for K,H,-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 206228 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACX, MAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.71	0/5257	0.73	1/7195 (0.0%)
1	B	0.69	0/5244	0.73	1/7178 (0.0%)
1	C	0.72	0/5254	0.75	1/7191 (0.0%)
1	D	0.72	1/5247 (0.0%)	0.74	0/7182
All	All	0.71	1/21002 (0.0%)	0.74	3/28746 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	325	CYS	CB-SG	-8.61	1.67	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	482	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	B	203	LEU	CB-CG-CD2	5.03	119.55	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5105	0	4917	35	0
1	B	5093	0	4891	26	0
1	C	5102	0	4912	35	0
1	D	5095	0	4889	21	0
2	A	66	0	60	1	0
2	B	66	0	60	1	0
2	C	66	0	60	1	0
2	D	66	0	60	2	0
3	A	23	0	22	1	0
3	B	23	0	22	3	0
3	C	23	0	22	1	0
3	D	23	0	22	1	0
4	A	127	0	0	5	0
4	B	111	0	0	2	0
4	C	120	0	0	3	0
4	D	101	0	0	1	0
All	All	21210	0	19937	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:VAL:HG13	1:A:629:PRO:HD2	1.46	0.94
1:B:395:ASN:HD21	3:B:703:MAL:C1'	1.86	0.89
1:C:617:MET:CE	1:C:622:LEU:HD12	2.06	0.85
1:A:628:VAL:HG13	1:A:629:PRO:CD	2.07	0.83
1:B:350:ALA:HB3	1:B:360:ILE:CD1	2.13	0.79
1:A:395:ASN:ND2	3:A:703:MAL:O5'	2.16	0.77
1:A:628:VAL:CG1	1:A:629:PRO:HD2	2.16	0.76
1:B:350:ALA:HB3	1:B:360:ILE:HD12	1.68	0.74
1:C:458:TYR:CE2	1:C:462:LEU:HD11	2.27	0.69
1:B:395:ASN:ND2	3:B:703:MAL:O5'	2.27	0.68
1:B:82:ALA:HB3	1:B:85:THR:HG21	1.77	0.66
1:A:628:VAL:CG1	1:A:629:PRO:CD	2.74	0.65
1:D:178:THR:HB	1:D:180:GLN:HE21	1.63	0.63
1:A:421:LEU:HD21	1:A:443:TYR:CE1	2.34	0.62
1:B:33:GLY:HA2	4:B:2005:HOH:O	1.98	0.62
1:A:18:VAL:HG12	1:A:19:GLY:O	2.00	0.61
1:C:617:MET:HE1	1:C:622:LEU:HD12	1.83	0.61
1:C:121:LYS:HD3	1:C:126:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD21	1:C:386:HIS:CE1	2.36	0.60
1:C:617:MET:HE3	1:C:617:MET:HA	1.84	0.59
1:C:445:TYR:CE1	2:C:701:ACX:H1F	2.38	0.58
1:D:240:PRO:HA	1:D:313:LEU:HD13	1.87	0.57
1:C:482:LEU:HD22	1:C:529:TYR:CD2	2.39	0.57
1:B:395:ASN:HD21	3:B:703:MAL:H1'	1.67	0.57
1:A:437:ILE:HD12	1:A:437:ILE:C	2.26	0.56
1:C:319:LEU:HD22	4:C:2061:HOH:O	2.06	0.56
1:C:395:ASN:ND2	3:C:703:MAL:O5'	2.40	0.55
1:B:67:ASP:HB2	1:B:68:PRO:CD	2.37	0.55
1:A:424:ALA:HB3	4:A:2092:HOH:O	2.06	0.55
1:C:582:LYS:HE3	1:C:610:GLU:O	2.08	0.54
1:C:67:ASP:HB2	1:C:68:PRO:CD	2.38	0.54
1:D:300:LEU:HD21	1:D:386:HIS:CE1	2.42	0.54
1:D:178:THR:HB	1:D:180:GLN:NE2	2.24	0.53
1:C:617:MET:HE2	1:C:622:LEU:HD12	1.90	0.52
1:A:180:GLN:O	1:A:184:VAL:HG23	2.09	0.52
1:B:495:GLU:O	1:B:499:VAL:HG23	2.09	0.52
1:A:67:ASP:HB2	1:A:68:PRO:CD	2.39	0.52
1:C:26:VAL:HG22	1:C:49:ALA:HB2	1.92	0.52
1:B:489:GLY:HA3	1:B:493:ALA:HB2	1.91	0.51
1:D:445:TYR:CE1	2:D:701:ACX:H1F	2.46	0.51
1:C:482:LEU:HD22	1:C:529:TYR:CE2	2.46	0.51
1:D:67:ASP:HB2	1:D:68:PRO:CD	2.39	0.51
1:D:155:LEU:O	1:D:159:VAL:HG23	2.11	0.51
1:A:500:LEU:CD1	4:A:2111:HOH:O	2.58	0.51
1:A:377:VAL:HG23	4:A:2088:HOH:O	2.10	0.50
1:D:489:GLY:HA3	1:D:493:ALA:HB2	1.94	0.49
1:C:178:THR:HB	1:C:180:GLN:HE21	1.77	0.49
1:D:178:THR:OG1	1:D:181:VAL:HG23	2.12	0.49
1:B:552:ILE:O	1:B:556:VAL:HG23	2.12	0.49
1:D:543:THR:HG23	4:D:2095:HOH:O	2.12	0.49
1:C:338:TRP:CD2	1:C:372:LEU:HD21	2.48	0.48
1:C:32:ARG:N	4:C:2009:HOH:O	2.28	0.48
1:A:146:VAL:O	1:A:152:ARG:NH2	2.41	0.48
1:B:300:LEU:HD21	1:B:386:HIS:CE1	2.48	0.48
1:C:617:MET:N	1:C:618:PRO:CD	2.77	0.48
1:A:482:LEU:HD22	1:A:529:TYR:CE2	2.50	0.47
1:D:395:ASN:ND2	3:D:703:MAL:O5'	2.47	0.47
1:A:489:GLY:HA3	1:A:493:ALA:HB2	1.97	0.47
1:D:608:THR:HA	1:D:651:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:O	1:D:152:ARG:NH2	2.42	0.46
1:A:399:LYS:N	1:A:399:LYS:HD2	2.31	0.46
1:C:23:VAL:HG21	1:C:104:VAL:HG12	1.98	0.46
1:B:282:ALA:HA	1:B:360:ILE:CG2	2.46	0.46
1:C:617:MET:CE	1:C:620:LEU:HD12	2.45	0.46
1:A:482:LEU:HD22	1:A:529:TYR:CD2	2.52	0.46
1:A:445:TYR:CE1	2:A:701:ACX:H1F	2.51	0.45
1:D:399:LYS:HD2	1:D:399:LYS:N	2.31	0.45
1:C:282:ALA:HA	1:C:360:ILE:CG2	2.46	0.45
1:D:621:GLY:O	1:D:622:LEU:HD23	2.16	0.45
1:B:608:THR:HA	1:B:651:PRO:HD3	1.98	0.45
1:C:489:GLY:HA3	1:C:493:ALA:HB2	1.98	0.45
1:A:617:MET:N	1:A:618:PRO:CD	2.80	0.45
1:A:30:VAL:HG12	1:A:31:GLN:HB2	1.98	0.45
1:A:437:ILE:HD12	1:A:438:GLY:N	2.32	0.45
1:C:82:ALA:HB3	1:C:85:THR:HG21	1.99	0.44
1:A:452:LYS:NZ	1:A:582:LYS:O	2.49	0.44
1:A:608:THR:HA	1:A:651:PRO:HD3	1.99	0.44
1:A:576:HIS:CG	1:A:619:GLN:HG2	2.53	0.44
1:B:445:TYR:CE1	2:B:701:ACX:H1F	2.52	0.44
1:B:617:MET:N	1:B:618:PRO:CD	2.80	0.44
1:B:338:TRP:CD2	1:B:372:LEU:HD21	2.53	0.44
1:A:500:LEU:HD12	4:A:2111:HOH:O	2.18	0.44
1:B:399:LYS:HD2	1:B:399:LYS:N	2.33	0.44
1:A:206:ARG:NH2	1:A:419:ILE:HD12	2.33	0.43
1:B:155:LEU:O	1:B:159:VAL:HG23	2.18	0.43
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.85	0.43
1:B:350:ALA:HB3	1:B:360:ILE:HD11	1.99	0.42
1:A:621:GLY:O	1:A:622:LEU:HD23	2.19	0.42
1:C:178:THR:HB	1:C:180:GLN:NE2	2.34	0.42
1:D:397:HIS:CD2	1:D:397:HIS:H	2.37	0.42
1:D:428:PRO:HD3	2:D:701:ACX:H2A	2.01	0.42
1:C:617:MET:HE1	1:C:620:LEU:HD12	2.02	0.42
1:D:617:MET:N	1:D:618:PRO:CD	2.82	0.42
1:C:276:ASP:HB3	4:C:2070:HOH:O	2.18	0.42
1:A:631:ARG:O	1:A:659:CYS:HA	2.20	0.42
1:B:67:ASP:HB2	1:B:68:PRO:HD2	2.02	0.42
1:A:437:ILE:CD1	1:A:437:ILE:C	2.88	0.41
1:A:567:PRO:HD3	4:A:2126:HOH:O	2.19	0.41
1:C:67:ASP:HB2	1:C:68:PRO:HD2	2.02	0.41
1:A:212:GLY:O	1:A:507:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LEU:HD23	1:D:313:LEU:HA	1.82	0.41
1:D:282:ALA:HA	1:D:360:ILE:CG2	2.51	0.41
1:B:68:PRO:HB3	4:B:2021:HOH:O	2.21	0.41
1:D:212:GLY:O	1:D:507:THR:HA	2.21	0.41
1:B:458:TYR:CE2	1:B:462:LEU:HD11	2.56	0.41
1:C:399:LYS:HD2	1:C:399:LYS:N	2.36	0.41
1:B:497:ARG:HA	1:B:497:ARG:HD2	1.92	0.41
1:B:238:ARG:HD2	1:B:238:ARG:HA	1.87	0.41
1:A:67:ASP:HB2	1:A:68:PRO:HD2	2.02	0.40
1:C:475:PHE:HA	1:C:509:GLY:O	2.21	0.40
1:C:578:HIS:HE2	1:C:589:SER:HB3	1.84	0.40
1:A:482:LEU:HD21	1:A:519:ASN:HA	2.03	0.40
1:C:294:HIS:ND1	1:C:295:PRO:HD2	2.36	0.40
1:C:176:ALA:O	1:C:177:LEU:HD23	2.21	0.40
1:B:423:GLU:HA	1:B:443:TYR:CD1	2.57	0.40
1:C:437:ILE:HD12	1:C:437:ILE:C	2.41	0.40
1:A:397:HIS:CD2	1:A:397:HIS:H	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	647/695 (93%)	634 (98%)	13 (2%)	0	100	100
1	B	647/695 (93%)	634 (98%)	13 (2%)	0	100	100
1	C	647/695 (93%)	631 (98%)	16 (2%)	0	100	100
1	D	647/695 (93%)	633 (98%)	14 (2%)	0	100	100
All	All	2588/2780 (93%)	2532 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	530/575 (92%)	520 (98%)	10 (2%)	65	77
1	B	526/575 (92%)	514 (98%)	12 (2%)	58	71
1	C	528/575 (92%)	513 (97%)	15 (3%)	51	63
1	D	526/575 (92%)	514 (98%)	12 (2%)	58	71
All	All	2110/2300 (92%)	2061 (98%)	49 (2%)	58	71

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	180	GLN
1	A	238	ARG
1	A	251	TYR
1	A	352	ASN
1	A	511	TYR
1	A	547	ARG
1	A	616	ASP
1	A	626	GLU
1	A	654	THR
1	B	31	GLN
1	B	180	GLN
1	B	238	ARG
1	B	251	TYR
1	B	270	LEU
1	B	352	ASN
1	B	511	TYR
1	B	547	ARG
1	B	616	ASP
1	B	626	GLU
1	B	637	GLU
1	B	654	THR
1	C	31	GLN
1	C	167	ARG

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Mol	Chain	Res	Type
1	C	180	GLN
1	C	238	ARG
1	C	251	TYR
1	C	270	LEU
1	C	323	LEU
1	C	352	ASN
1	C	511	TYR
1	C	547	ARG
1	C	582	LYS
1	C	616	ASP
1	C	626	GLU
1	C	637	GLU
1	C	654	THR
1	D	31	GLN
1	D	121	LYS
1	D	238	ARG
1	D	251	TYR
1	D	270	LEU
1	D	352	ASN
1	D	511	TYR
1	D	547	ARG
1	D	616	ASP
1	D	626	GLU
1	D	637	GLU
1	D	654	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	A	397	HIS
1	A	436	GLN
1	B	56	HIS
1	B	262	HIS
1	B	395	ASN
1	B	436	GLN
1	C	180	GLN
1	C	397	HIS
1	C	436	GLN
1	D	180	GLN
1	D	262	HIS
1	D	397	HIS

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Mol	Chain	Res	Type
1	D	436	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACX	A	701	-	72,72,72	0.51	0	108,108,108	1.06	6 (5%)
3	MAL	A	703	-	24,24,24	0.91	1 (4%)	35,35,35	1.99	11 (31%)
2	ACX	B	701	-	72,72,72	0.65	0	108,108,108	1.21	12 (11%)
3	MAL	B	703	-	24,24,24	0.75	1 (4%)	35,35,35	1.92	10 (28%)
2	ACX	C	701	-	72,72,72	0.64	0	108,108,108	1.20	12 (11%)
3	MAL	C	703	-	24,24,24	0.95	1 (4%)	35,35,35	1.83	9 (25%)
2	ACX	D	701	-	72,72,72	0.56	0	108,108,108	1.04	6 (5%)
3	MAL	D	703	-	24,24,24	0.60	0	35,35,35	1.94	12 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACX	A	701	-	-	0/36/156/156	0/0/7/7
3	MAL	A	703	-	-	0/8/48/48	0/2/2/2
2	ACX	B	701	-	-	0/36/156/156	0/0/7/7
3	MAL	B	703	-	-	0/8/48/48	0/2/2/2
2	ACX	C	701	-	-	0/36/156/156	0/0/7/7
3	MAL	C	703	-	-	0/8/48/48	0/2/2/2
2	ACX	D	701	-	-	0/36/156/156	0/0/7/7
3	MAL	D	703	-	-	0/8/48/48	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	MAL	O1-C4'	-2.28	1.38	1.43
3	C	703	MAL	O1-C1	2.01	1.47	1.41
3	B	703	MAL	O3'-C3'	2.08	1.47	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	MAL	O5'-C1'-C2'	-5.40	101.19	109.80
3	B	703	MAL	C2'-C3'-C4'	-3.82	101.22	109.60
3	C	703	MAL	O5'-C1'-C2'	-3.76	103.80	109.80
3	A	703	MAL	C1-C2-C3	-3.75	102.58	109.97
3	D	703	MAL	O5'-C5'-C6'	-3.65	97.14	106.36
3	B	703	MAL	C1-O1-C4'	-3.54	108.74	118.01
3	C	703	MAL	O3'-C3'-C2'	-3.50	102.45	110.34
3	C	703	MAL	C1-O1-C4'	-3.45	108.98	118.01
3	D	703	MAL	C1-O1-C4'	-3.41	109.10	118.01
3	A	703	MAL	O5'-C1'-C2'	-3.35	104.46	109.80
3	B	703	MAL	O5'-C1'-C2'	-3.28	104.57	109.80
3	A	703	MAL	O1-C4'-C5'	-3.09	101.20	109.32
3	A	703	MAL	C1-O5-C5	-3.03	107.87	113.75
3	D	703	MAL	O2-C2-C1	-2.51	104.52	110.02
2	B	701	ACX	O1A-C4B-C3B	-2.48	100.77	107.17
2	B	701	ACX	O3F-C3F-C2F	-2.28	105.19	110.34
3	B	703	MAL	C6'-C5'-C4'	-2.22	106.78	113.25
3	B	703	MAL	O3-C3-C4	-2.19	105.40	110.34
3	D	703	MAL	O3'-C3'-C2'	-2.16	105.48	110.34
3	D	703	MAL	O4-C4-C3	-2.13	105.54	110.34
2	C	701	ACX	O5A-C1A-C2A	-2.09	105.98	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ACX	O5C-C1C-C2C	-2.07	106.03	110.28
3	A	703	MAL	C6'-C5'-C4'	-2.05	107.28	113.25
3	D	703	MAL	O2'-C2'-C3'	2.00	114.85	110.34
3	B	703	MAL	O3-C3-C2	2.04	114.93	110.34
2	C	701	ACX	O5C-C5C-C6C	2.07	111.59	106.36
2	B	701	ACX	C3B-C4B-C5B	2.08	115.54	110.84
3	A	703	MAL	O5-C5-C6	2.10	111.66	106.36
3	C	703	MAL	O2'-C2'-C1'	2.12	114.48	109.82
2	B	701	ACX	O5F-C5F-C6F	2.12	111.72	106.36
3	D	703	MAL	C1-C2-C3	2.12	114.16	109.97
2	C	701	ACX	C1C-C2C-C3C	2.14	114.19	109.97
2	D	701	ACX	O1B-C1B-C2B	2.14	113.32	108.10
2	B	701	ACX	C3F-C4F-C5F	2.16	115.72	110.84
3	A	703	MAL	O2-C2-C1	2.19	114.83	110.02
2	A	701	ACX	O5B-C5B-C4B	2.20	114.39	109.75
2	C	701	ACX	O5F-C5F-C6F	2.22	111.97	106.36
2	D	701	ACX	O2A-C2A-C3A	2.22	115.35	110.34
3	C	703	MAL	C1-C2-C3	2.23	114.36	109.97
3	A	703	MAL	O2-C2-C3	2.23	115.36	110.34
2	C	701	ACX	O1B-C1B-C2B	2.24	113.56	108.10
2	D	701	ACX	C3C-C4C-C5C	2.25	115.93	110.84
3	D	703	MAL	O2'-C2'-C1'	2.29	114.87	109.82
2	B	701	ACX	C1D-O5D-C5D	2.30	118.21	113.75
2	A	701	ACX	C3E-C4E-C5E	2.37	116.19	110.84
2	A	701	ACX	C3C-C4C-C5C	2.37	116.19	110.84
3	D	703	MAL	O5-C5-C4	2.40	114.19	109.68
3	A	703	MAL	O5-C1-C2	2.46	115.32	110.28
2	C	701	ACX	O1F-C1F-O5F	2.47	116.93	110.68
2	D	701	ACX	O5A-C5A-C4A	2.50	115.03	109.75
2	A	701	ACX	C1B-O5B-C5B	2.52	118.64	113.75
2	D	701	ACX	C1A-O5A-C5A	2.52	118.64	113.75
3	D	703	MAL	O1-C4'-C3'	2.60	113.88	107.17
2	B	701	ACX	O1C-C1C-C2C	2.65	114.56	108.10
2	C	701	ACX	C2E-C3E-C4E	2.68	115.48	109.60
2	D	701	ACX	C2C-C3C-C4C	2.71	115.54	109.60
2	B	701	ACX	O5E-C5E-C4E	2.73	115.51	109.75
3	C	703	MAL	O1-C4'-C3'	2.74	114.25	107.17
2	C	701	ACX	C3E-C4E-C5E	2.78	117.11	110.84
2	A	701	ACX	O5E-C5E-C4E	2.78	115.63	109.75
3	B	703	MAL	O3'-C3'-C4'	2.80	116.49	109.87
2	A	701	ACX	C2C-C3C-C4C	2.80	115.76	109.60
2	B	701	ACX	O5C-C5C-C4C	2.82	115.70	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	ACX	O5D-C5D-C4D	2.86	115.78	109.75
2	C	701	ACX	C2C-C3C-C4C	2.86	115.88	109.60
2	B	701	ACX	O5A-C5A-C6A	2.86	113.58	106.36
3	C	703	MAL	O3'-C3'-C4'	2.93	116.80	109.87
3	C	703	MAL	O1'-C1'-C2'	2.94	117.09	109.21
3	B	703	MAL	O1-C4'-C3'	3.08	115.12	107.17
2	C	701	ACX	C1D-O5D-C5D	3.09	119.74	113.75
3	A	703	MAL	O1-C1-C2	3.15	115.76	108.10
3	B	703	MAL	C1'-O5'-C5'	3.21	119.41	113.47
2	C	701	ACX	O1F-C4A-C3A	3.28	115.63	107.17
3	C	703	MAL	C1'-O5'-C5'	3.37	119.70	113.47
2	B	701	ACX	C1C-O5C-C5C	3.64	120.80	113.75
3	B	703	MAL	O5'-C5'-C4'	4.08	118.36	109.75
3	D	703	MAL	O1'-C1'-C2'	4.08	120.15	109.21
3	A	703	MAL	O1-C1-O5	4.86	122.99	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ACX	1	0
3	A	703	MAL	1	0
2	B	701	ACX	1	0
3	B	703	MAL	3	0
2	C	701	ACX	1	0
3	C	703	MAL	1	0
2	D	701	ACX	2	0
3	D	703	MAL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	649/695 (93%)	-0.54	1 (0%) 95 95	21, 31, 51, 69	0
1	B	649/695 (93%)	-0.51	0 100 100	17, 29, 56, 82	0
1	C	649/695 (93%)	-0.48	0 100 100	18, 32, 51, 70	0
1	D	649/695 (93%)	-0.47	1 (0%) 95 95	18, 31, 55, 66	0
All	All	2596/2780 (93%)	-0.50	2 (0%) 95 95	17, 31, 54, 82	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PRO	2.5
1	D	644	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACX	D	701	66/66	0.87	0.23	16.57	49,85,119,124	0
2	ACX	C	701	66/66	0.89	0.17	6.60	41,68,89,93	0
2	ACX	A	701	66/66	0.91	0.15	5.08	41,69,81,84	0
2	ACX	B	701	66/66	0.93	0.14	2.75	36,57,75,84	0
3	MAL	D	703	23/23	0.95	0.09	0.22	22,25,37,42	0
3	MAL	C	703	23/23	0.96	0.09	-0.10	22,26,34,36	0
3	MAL	B	703	23/23	0.96	0.09	-0.49	21,25,30,33	0
3	MAL	A	703	23/23	0.96	0.08	-0.67	23,29,34,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.